

Motivation

Fluid flow coupled with deformable solid particles has many applications in biological and engineering problems, e.g., blood cell transport, drug delivery, blood clotting. We present a partitioned approach to solve the coupled Multiphysics problem. The fluid motion was solved by **PALABOS (parallel Lattice Boltzmann solver)**, while the solid displacement and deformation was simulated by **LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator)**. The coupling was achieved through the **immersed boundary method**. The code can model both **rigid** and **deformable** solids. The code also showed great scaling results over 8192 processors, highlighting the capabilities of the code.

Methods

Fluid: Lattice Boltzmann method (PALABOS)

Dynamics of distribution functions

$$\underbrace{f_i(x + \Delta t \vec{c}_i, t + \Delta t) - f_i(x, t)}_{\text{Streaming}} = \underbrace{\Omega_i + F_i}_{\text{Collision}}$$

$$\Omega_i = \frac{1}{\tau} (f_i(x, t) - f_i^{eq}(x, t)) \quad F_i = (1 - \frac{1}{2\tau}) w_i \left(\frac{\vec{c}_i \cdot \vec{u}}{c_s^2} + \frac{\vec{c}_i \cdot \vec{u}}{c_s^4} \right) \cdot \vec{f}$$

Solid: cell membrane model (LAMMPS)

Stretching. Bending. Area/Volume conservation energy

$$V(\{\mathbf{x}_i\}) = V_{in-plane} + V_{bending} + V_{area} + V_{volume}$$

$$V_{stretch} = \sum_{j=1 \dots N_s} \left[\frac{k_B T l_m}{4p} \frac{3x_j^2 - 2x_j^3}{1 - x_j} + \frac{k_p}{l_j} \right] \quad V_{bending} = \sum_{j=1 \dots N_s} k_b (1 - \cos(\theta_j - \theta_0))$$

Coupling: Immersed boundary method

Force and velocity continuous over the interface

$$\mathbf{f}(\mathbf{x}, t) = \int \mathbf{F}(s, t) \delta(\mathbf{x} - \mathbf{X}(s, t)) ds \quad \mathbf{u}(\mathbf{X}, t) = \int \mathbf{u}(\mathbf{x}, t) \delta(\mathbf{x} - \mathbf{X}(s, t)) d\mathbf{x}$$

$$\text{Force coupling } F^{fsi} = \rho_f (U_f - U_s) / \Delta t$$

• Solid nodes (X) ■ Fluid nodes (x)

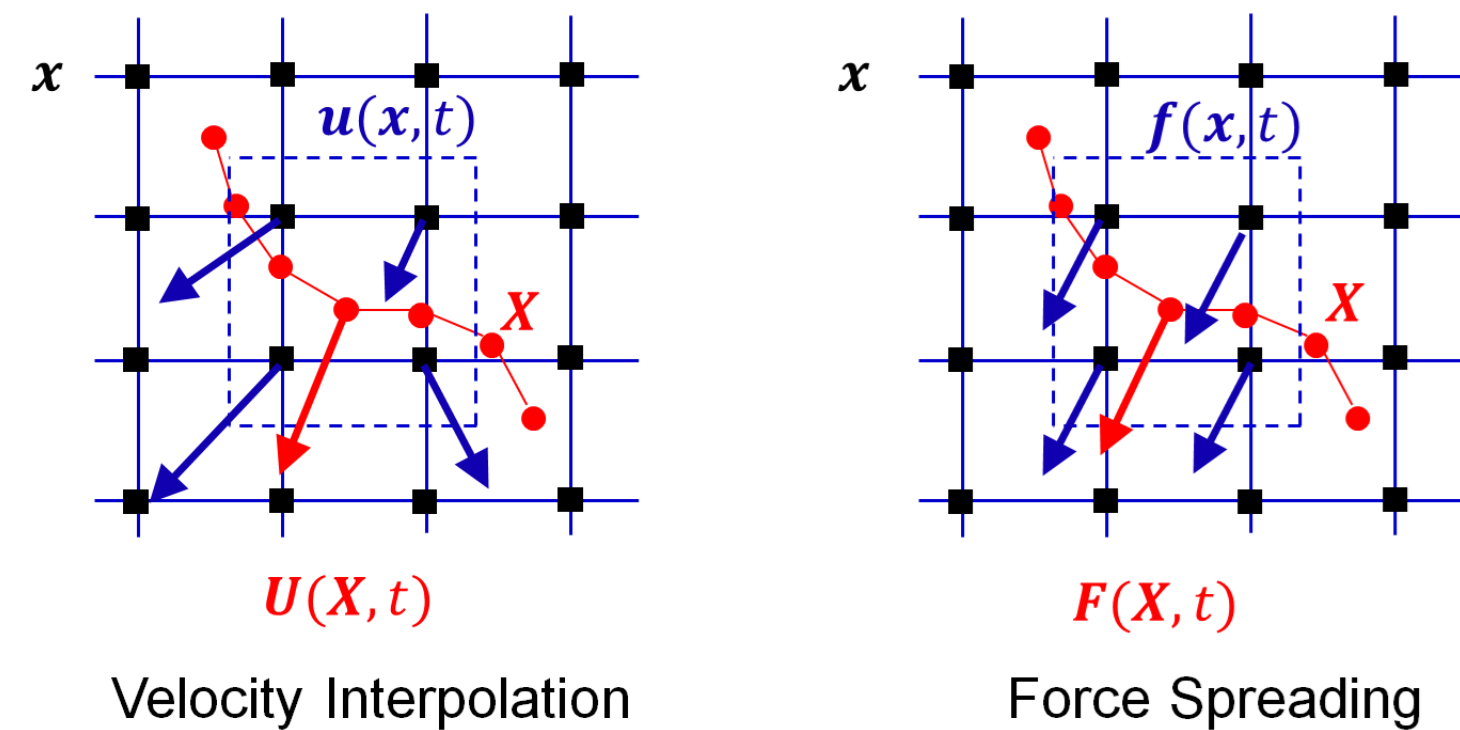


Fig. 1. The spreading of solid force into local fluid grids. The interpolation of solid velocity from local fluid velocity

Validations

a. Ellipsoid orbit under shear flow

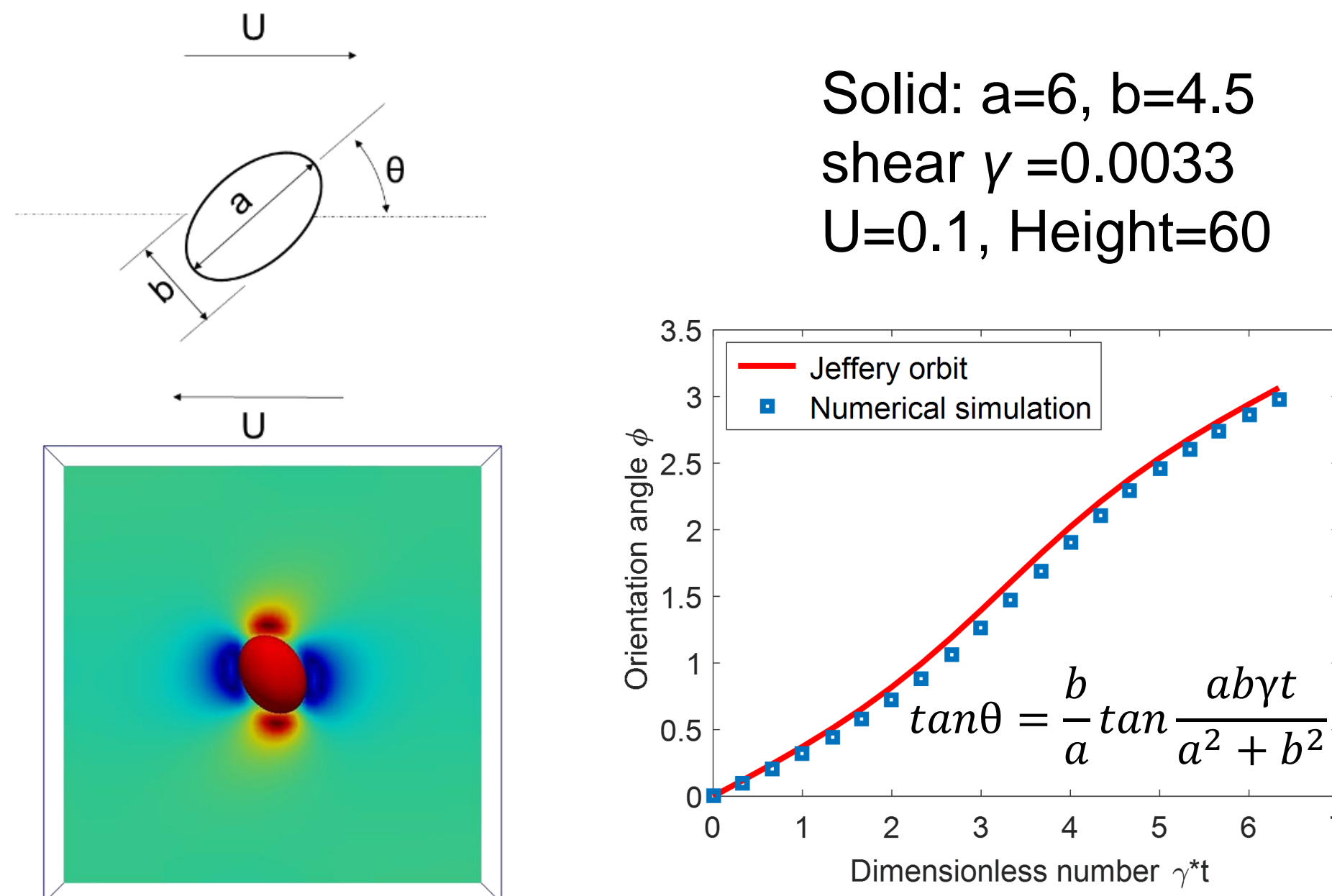


Fig.2. Jeffery's orbit for an ellipsoid under shear flow

b. Red blood cell: optical tweezer stretching test

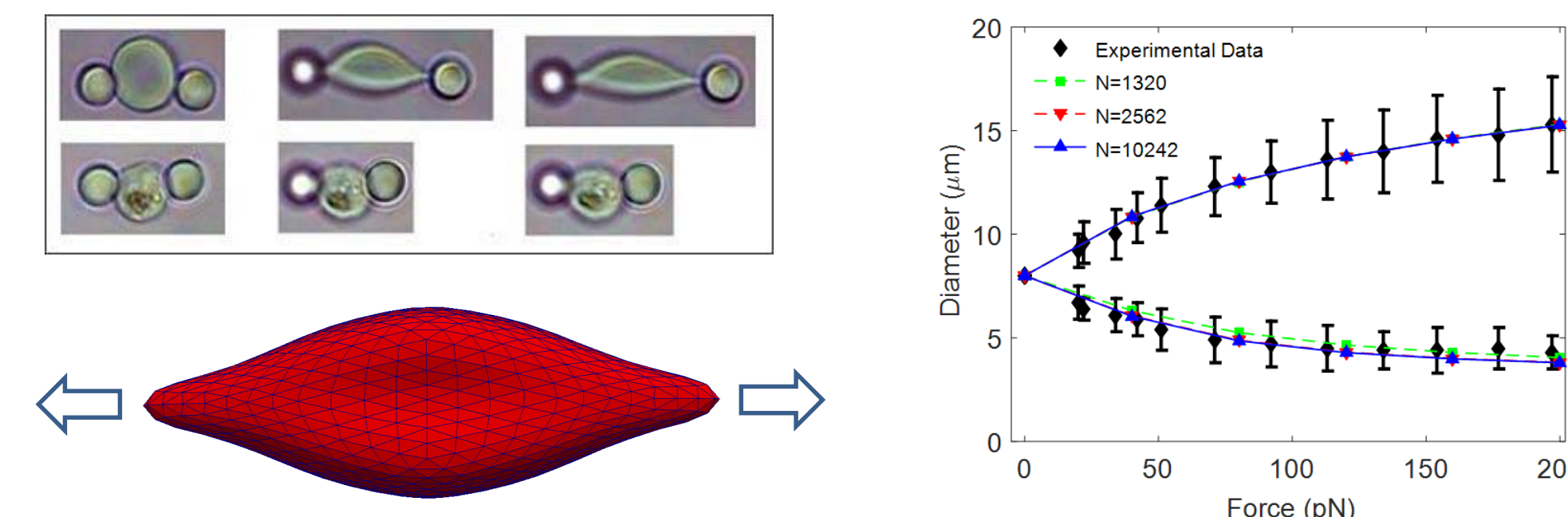


Fig. 3. The comparison of simulation with experiments for red blood cell stretching

c. Blood effective viscosity in different tubes

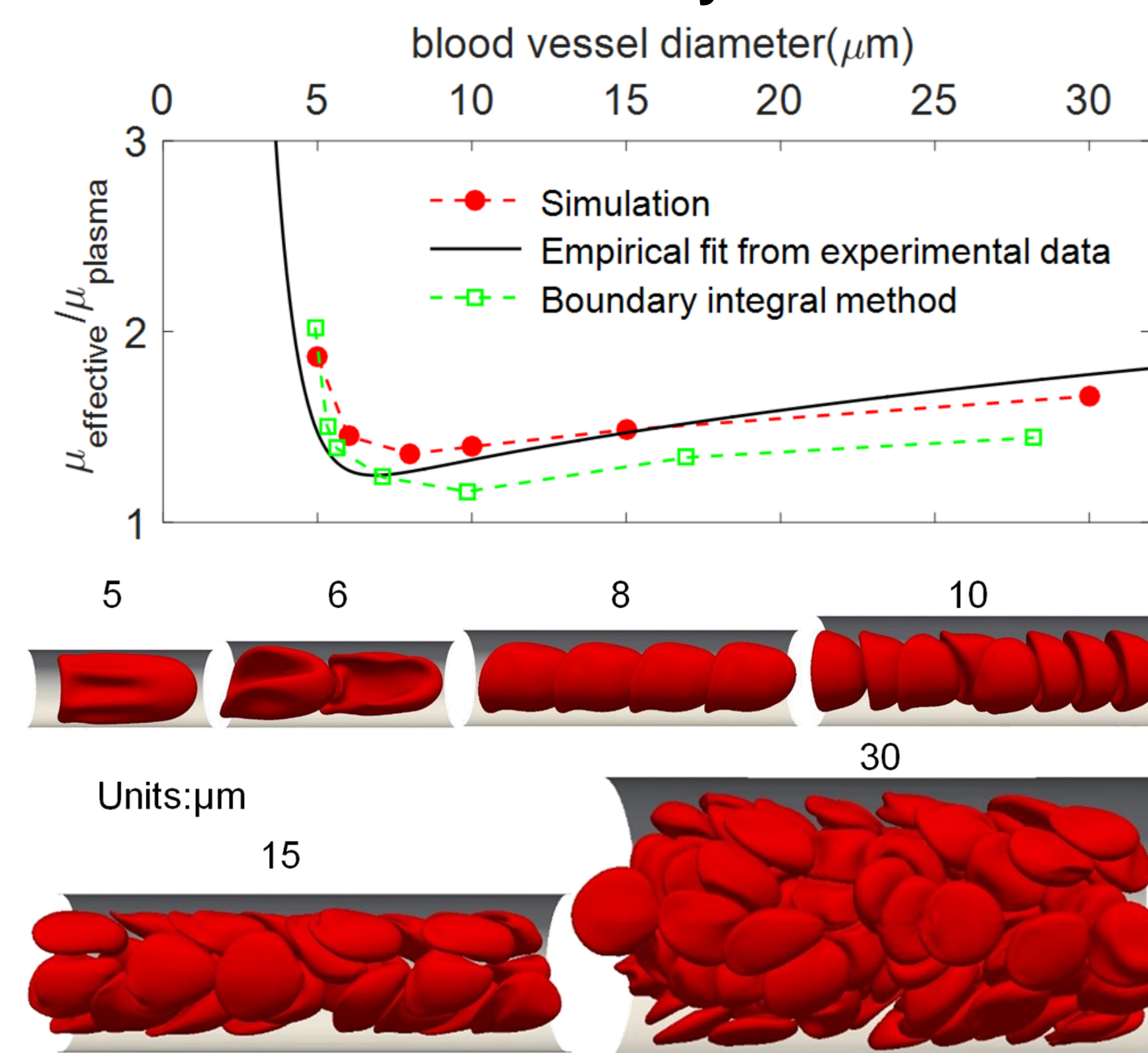


Fig. 4. The effective viscosity of blood flowing through different tube sizes.

Performance

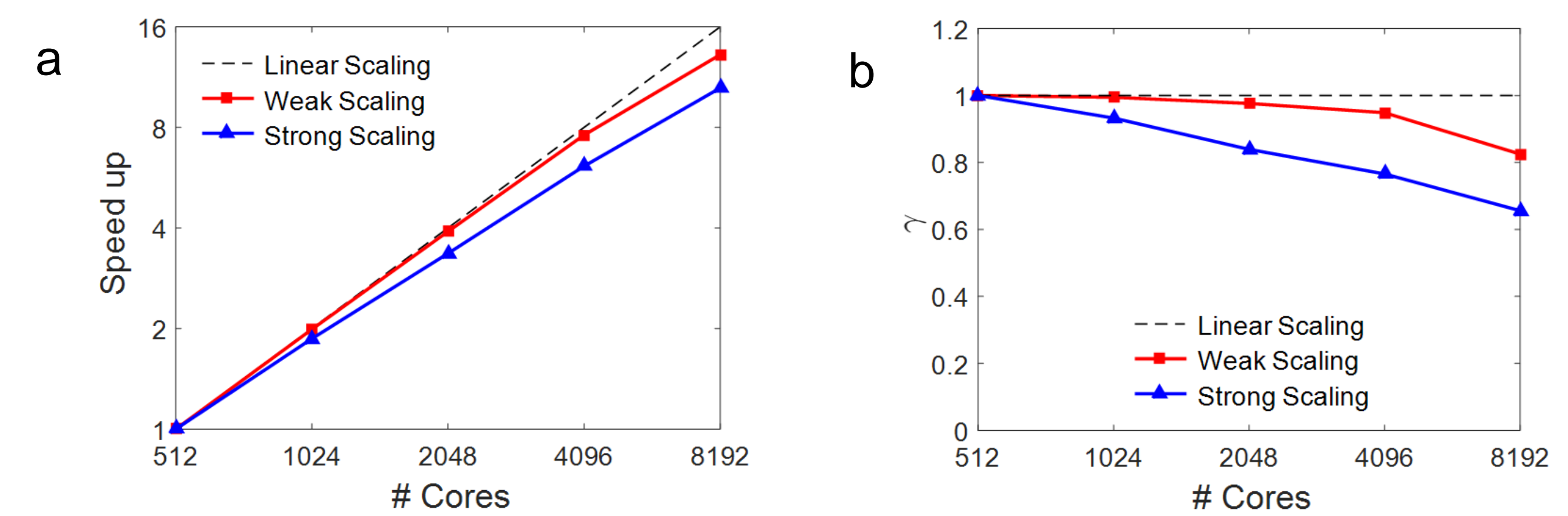


Fig.5. The performance of the code over thousands of processors. The system consists of 20,697,600 solid particles, 93,312,000 fluid nodes. (a) The speed up. (b) The scaling efficiency.

Applications

Filament transport in blood cell suspensions

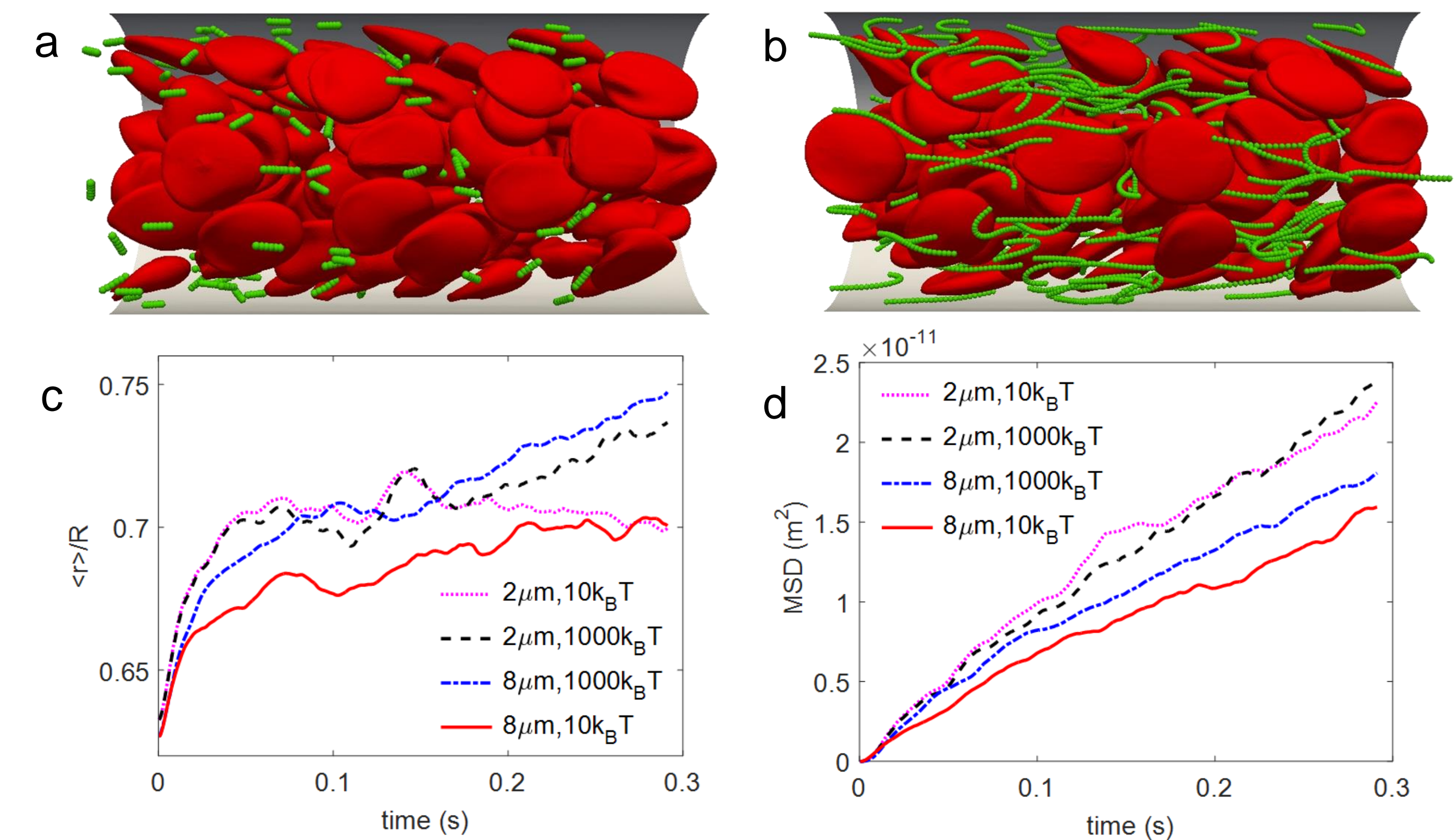


Fig. 6. The size and flexibility effect on the filaments transport in blood cell suspensions was simulated. The transport of filaments (green) mixing with red blood cells (red) in a cylindrical channel (R,L = 15,50 um). The snapshots of the simulation for (a) 2 um filaments; (b) 8 um filaments; (c) The averaged the particle position in the channel; (d) The mean square displacement of the particles.

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The simulation was performed on GAEA from NIU and Mira at the Argonne National Laboratory.

Reference: J. Tan, T. Sinno, S. Diamond, J. Comput. Sci.25 (2018) 89–100